

Adaptive logarithmic discretization for numerical renormalization group methods

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Abstract

The problem of the logarithmic discretization of an arbitrary positive function (such as the density of states) is studied in general terms. Logarithmic discretization has arbitrary high resolution around some chosen point (such as Fermi level) and it finds application, for example, in the numerical renormalization group (NRG) approach to quantum impurity problems (Kondo model), where the continuum of the conduction band states needs to be reduced to a finite number of levels with good sampling near the Fermi level. The discretization schemes under discussion are required to reproduce the original function after averaging over different interleaved discretization meshes, thus systematic deviations which appear in the conventional logarithmic discretization are eliminated. An improved scheme is proposed in which the discretization-mesh points themselves are determined in an adaptive way; they are denser in the regions where the function has higher values. Such schemes help in reducing the residual numeric artefacts in NRG calculations in situations where the density of states approaches zero over extended intervals. A reference implementation of the solver for the differential equations which determine the full set of discretization coefficients is also described.

Key words: logarithmic discretization, adaptive meshing, numerical renormalization group

1. Introduction

Discretization of the continuum of conduction-band electron states to a finite set of levels is a common approximation procedure in many practical problems in computational condensed-matter physics. In band structure calculations, for example, the discretization is performed in the reciprocal space where a finite number of judiciously chosen (symmetry-adapted) crystal-momentum points are chosen to sample contributions from various regions of the full Brillouin zone [1]. Various real-space approaches based on finite-difference or finite-element formulations are also possible [2]. Finally, in the numerical renormalization group (NRG) methods for solving quantum impurity problems the quantity that is discretized is the density of states, thus the discretization is effectively performed in the energy space [3, 4, 5, 6]. In order to obtain good sampling of states near the Fermi level, the discretization mesh consists of a geometric series of points, so that very high resolution is achieved in the vicinity of the Fermi level [3]; this choice is motivated by the nature of the quantum impurity problems (described by models such as the Kondo model or the Anderson impurity model), where excitations from different energy scales have a comparable effect on the physical properties. NRG allows to calculate dynamic properties (spectral functions, dynamic susceptibilities) of impurity models [7, 8, 9, 10, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20] and, in particular, it may be used as an impurity solver in the dynamic mean-field theory (DMFT) approach to the strongly-correlated electron systems [21, 22, 23, 24, 25, 26]. Logarithmic discretization of the conductance band can also be

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used in the density-matrix renormalization-group (DMRG) calculations [27, 28, 29], in the embedded-cluster approximation [30], and in the artificial Friedel resonance approach [31].

Recent work has revealed that the conventional discretization schemes used in NRG lead to discretization artefacts, which restrain the accuracy of calculations and limit the ultimate resolution that may be achieved [20]. A new approach to the discretization based on requiring exact reproduction of the conduction-band density of states (after discretization-mesh averaging) was shown to lead to a notable reduction of the artefacts [20]. In this paper the approach is further improved by making the discretization grid itself adaptable. This work is organized as follows: in Sec. 2 the discretization problem is formulated in very general terms starting from basic principles in order to determine the most general form of the discretization equations. In Sec. 3, the origin of the residual artefacts in the fixed-discretization-mesh approach is studied, while Sec. 4 presents a simple way of adapting the discretization grid to the density of states. Finally, in Sec. 5 the implementation of the discretization equation solver is described.

2. Problem statement

We consider a non-interacting Hamiltonian for the conductance-band electrons describing a set of N states indexed by some quantum number k :

$$H = \sum_{k=1}^N \epsilon_k |k\rangle \langle k|. \quad (1)$$

We assume that for all k , $\epsilon_k \in [-D : D]$, and in the following we use D as the unit of energy. The density of states at energy ω is defined as

$$\rho(\omega) = \frac{1}{N} \sum_k \delta(\omega - \epsilon_k), \quad (2)$$

and it is normalized to 1. In the continuum $N \rightarrow \infty$ limit, $\rho(\omega)$ is an arbitrary positive function with finite support $[-1 : 1]$. Our goal is to find a discrete representation of the continuum of states that is suitable for numeric calculations in quantum impurity physics and which reproduces the density of states $\rho(\omega)$ as accurately as possible. The approach is clearly applicable to an arbitrary positive function (in the single-impurity Anderson model, for example, the function of interest is the hybridisation function Γ), but to be specific we may think of it as a density of states.

In the following we focus on positive energies ω ; for negative ω the procedure is fully equivalent. We discretize the interval $[0 : 1]$ by defining the discretization-mesh points ϵ_j , $j \in \mathbb{N}$, such that

$$\epsilon_1 = 1, \quad \epsilon_j > \epsilon_{j+1}, \quad \lim_{j \rightarrow \infty} \epsilon_j = 0. \quad (3)$$

In order to achieve high resolution near $\omega = 0$ (i.e. in the vicinity of the Fermi level), we furthermore require that ϵ_j behave asymptotically as

$$\epsilon_j \sim \Lambda^{-j}, \quad (4)$$

where $\Lambda > 1$ is a constant number known as the discretization parameter. We denote each discretization interval $[\epsilon_{j+1} : \epsilon_j]$ as I_j . Within each interval I_j we choose a representative energy \mathcal{E}_j . Approximating $\mathcal{E}_j \approx \epsilon_j$, we see that the relative “resolution”

$$\frac{\Delta E}{E} \approx \frac{E_j - E_{j+1}}{E_j + E_{j+1}} \approx \frac{\Lambda - 1}{\Lambda + 1} \quad (5)$$

is approximately the same on all energy scales; from this property stems the name “logarithmic discretization”. We furthermore notice that the resolution is improved as Λ is reduced toward $\Lambda = 1$, which corresponds to returning to the continuum limit. At given Λ greater than 1, however, the continuum spectral density is represented by a set of delta peaks,

$$\tilde{\rho}(\omega) = \sum_j w_j \delta(\omega - \mathcal{E}_j), \quad \text{for } \omega > 0, \quad (6)$$

where weights w_j need to be chosen so that the normalization is preserved:

$$\sum_{j=1}^{\infty} w_j = \int_0^{\infty} \rho(\omega) d\omega = W. \quad (7)$$

Here we have introduced the total spectral weight for positive frequencies, W . The prescription for determining the discretization-mesh points ϵ_j , representative energies \mathcal{E}_j and weights w_j (and their negative-frequency analogues ϵ_j^- , \mathcal{E}_j^- , and w_j^-) is what we refer to as a “discretization scheme”. Several such procedures are known from the literature on the numerical renormalization group [3, 9, 32, 33, 34, 35, 36, 37, 16, 20].

A commonly used technique to improve the accuracy of numerical calculations is to perform computations for several different discretizations of the continuum and average the results. In the context of the numerical renormalization group, this is known as the “ z -averaging” or the “interleaved method” [9, 32, 16]. In this approach one introduces a continuous parameter $z \in [0 : 1]$ which characterizes different discretizations $\{\epsilon_j^z, \mathcal{E}_j^z, w_j^z\}$. Parameter z is sometimes called the “twist parameter” since it can be related to twisting the boundary conditions of the wave-functions of the conduction-band electrons [16]. The z -averaging procedure is meaningful when the boundary conditions

$$\forall z \quad \epsilon_1^z = 1, \quad \mathcal{E}_1^0 = 1, \quad (8)$$

and continuity constraints

$$\forall j \quad \epsilon_j^1 = \epsilon_{j+1}^0, \quad \forall j \quad \mathcal{E}_j^1 = \mathcal{E}_{j+1}^0, \quad (9)$$

are satisfied. We also require that ϵ_j^z and \mathcal{E}_j^z be monotonously decreasing functions of z , but they need not be continuous. Furthermore, for each value of z , the weights need to be normalized:

$$\sum_{j=1}^{\infty} w_j^z = W. \quad (10)$$

The spectral density is then determined as the average (integral) over z [16]:

$$A(\omega) = \int_0^1 \tilde{\rho}(z, \omega) dz, \quad (11)$$

where $\tilde{\rho}(z, \omega)$ is given by the generalization of Eq. (6):

$$\tilde{\rho}(z, \omega) = \sum_j w_j^z \delta(\omega - \mathcal{E}_j^z). \quad (12)$$

We obtain [16]

$$A(\omega) = \sum_j \int_0^1 w_j^z \delta(\omega - \mathcal{E}_j^z) dz = \frac{w_j^z}{-\partial \mathcal{E}_j^z / \partial z}, \quad (13)$$

where the parameters j and z in the last part of the expression are determined implicitly through the relation $\omega = \mathcal{E}_j^z$; this choice of j and z is unique due to the requirement that \mathcal{E}_j^z is strictly decreasing as a function of z . In practical calculations, only a small number N_z of values of z is used (often as small as 4 or 2, or even a single one) and the integral is approximated using the rectangle method; the resulting function then needs to be broadened appropriately to obtain a continuous representation. See, however, Ref. [20] for calculations with a large N_z and very narrow broadening kernel, which show that overbroadening errors of NRG can largely be eliminated.

To simplify the notation and to provide more insight into the mathematical structure of the problem, we introduce continuous indexing of the discretization-grid points as [20]

$$x = j + z. \quad (14)$$

The “grid parameter” x runs from 1 to $+\infty$ and the coefficients ϵ_j^z , \mathcal{E}_j^z and w_j^z become continuous functions $\epsilon(x)$, $\mathcal{E}(x)$ and $w(x)$, while the continuity constraints, Eq. (9), are automatically satisfied. Both $\epsilon(x)$ and $\mathcal{E}(x)$ are required to be monotonously decreasing and, furthermore, the following boundary conditions need to be satisfied:

$$\epsilon(x) = 1 \text{ for } x \leq 2, \quad \lim_{x \rightarrow \infty} \epsilon(x) = 0, \quad (15)$$

$$\mathcal{E}(1) = 1, \quad \lim_{x \rightarrow \infty} \mathcal{E}(x) = 0. \quad (16)$$

These equations embody the requirement that as the grid parameter x sweeps the interval $[1 : +\infty)$, both the grid energy $\epsilon(x)$ and the representative energy $\mathcal{E}(x)$ describe the totality of the unit interval $[0 : 1]$. For convenience, we define the inverse function R to \mathcal{E} as $x = R(\omega)$, i.e. $R \circ \mathcal{E} = 1$.

Using newly introduced notation, Eq. (13) becomes

$$A(\omega) = \frac{w(x)}{-d\mathcal{E}(x)/dx}, \text{ with } x = R(\omega). \quad (17)$$

The normalization condition can be expressed as

$$\int_0^1 A(\omega) d\omega = \int_{-\infty}^1 A(\omega) \frac{d\mathcal{E}(x)}{dx} dx = \int_1^{\infty} w(x) dx = W, \quad (18)$$

but, in addition, the more general normalization equation

$$\sum_{j=1}^{\infty} w(j+z) = W, \quad (19)$$

which follows from Eq. (10), must be satisfied for each $z \in [0 : 1]$; in fact, Eq. (18) follows trivially from Eq. (19). We notice that the function $\epsilon(x)$ appears neither in Eq. (17) nor in Eq. (19); grid coefficients $\epsilon(x)$ are thus only auxiliary quantities which define the discretization grid without actually explicitly appearing in the final result for the density of states.

With all these preparations we can now finally state the problem as follows: we seek to determine functions $\mathcal{E}(x)$ and $w(x)$ such that

$$\frac{w[R(\omega)]}{-d\mathcal{E}[R(\omega)]/dx} = \rho(\omega), \quad (20)$$

and satisfying normalisation, Eq. (19).

Since, $\epsilon(x) = 1$ for $x \in [1 : 2]$ and $\epsilon(x) \rightarrow 0$ as $x \rightarrow \infty$, it is easy to see that $w(x)$ defined as

$$w(x) = \int_{\epsilon(x+1)}^{\epsilon(x)} \rho(\omega) d\omega \quad (21)$$

solves the normalization Eq. (19). In fact, this is the only general solution of Eq. (19); we note, however, that $\epsilon(x)$ can in principle still be an arbitrary monotonously decreasing function on the interval $[2 : \infty)$. Thus $w(x)$ *must* be defined as the integral of the density of states in the discretization integral $I(x) = [\epsilon(x+1) : \epsilon(x)]$, while we still have the full liberty of choosing the discretization mesh in any convenient way.

To make contact with the original motivation for introducing the logarithmic discretization of a continuum, we now focus on discretization meshes $\epsilon(x)$ with asymptotic behavior $\epsilon(x) \sim \Lambda^{2-x}$, where we have shifted the exponent by 2 for convenience. This asymptotic form is equivalent to requiring

$$\frac{d\epsilon(x)}{dx} = -\Lambda^{2-x} \ln \Lambda C(x, \epsilon), \quad (22)$$

where $C(x, \epsilon)$ is an arbitrary strictly positive function with a non-zero limit

$$\lambda = \lim_{\substack{x \rightarrow \infty \\ \epsilon \rightarrow 0}} C(x, \epsilon). \quad (23)$$

The requirement $\lambda \neq 0$ is necessary to obtain the desired asymptotic behavior.

The problem is thus reduced to finding an appropriate function $C(x, \epsilon)$. Once $C(x, \epsilon)$ is chosen, the full solution of the problem is obtained by solving the initial value problem

$$\begin{aligned} \mathcal{E}(1) &= 1, \\ \frac{d\mathcal{E}(x)}{dx} &= -\frac{\int_{\epsilon(x+1)}^{\epsilon(x)} \rho(\omega) d\omega}{\rho[\mathcal{E}(x)]}. \end{aligned} \quad (24)$$

In NRG, the discrete levels resulting from the discretization for given twist parameter z are used to write the discretized form of the conduction-band Hamiltonian

$$H = \sum_{i=1}^{\infty} \mathcal{E}_i^z |i\rangle \langle i|. \quad (25)$$

One then forms the combination of levels

$$|f_0\rangle = \sum_i \sqrt{w_i} |i\rangle, \quad (26)$$

and transforms the Hamiltonian H into a new basis (the first state of which is $|f_0\rangle$), so that the Hamiltonian takes the form of a tight-binding chain [3, 5, 38, 6]:

$$H = \sum_{n=0}^{\infty} \xi_n |f_n\rangle \langle f_n| + \sum_{n=0}^{\infty} t_n (|f_n\rangle \langle f_{n+1}| + |f_{n+1}\rangle \langle f_n|). \quad (27)$$

This form is known as the “hopping Hamiltonian” or the “Wilson chain”. The coefficients t_n decrease asymptotically as $t_n \propto \Lambda^{-n/2}$ and only a finite number of chain sites is retained in practical NRG calculations. The impurity hybridizes with the conduction band through level $|f_0\rangle$ only; this implies that the spectral function $A_f(\omega)$ of the level f_0 represents the density of states of the conduction band as seen by the impurity. The goal is thus to make $A_f(\omega)$ a good representation of the density of states $\rho(\omega)$.

We will discuss possible choices of $C(x, \epsilon)$ in Sec. 4 and describe a numerical approach for solving the initial value problem in Sec. 5, but we first pause to describe the previously known discretization schemes based on fixed discretization mesh to point out the origin of their deficiencies.

3. Fixed discretization mesh

The conventional logarithmic discretization used in NRG calculations is based on the fixed discretization mesh obtained by setting $C(x, \epsilon) \equiv 1$ in Eq. (22), with solution

$$\epsilon(x) = \begin{cases} 1 & \text{for } x \in [1 : 2], \\ \Lambda^{2-x} & \text{for } x \geq 2. \end{cases} \quad (28)$$

The different discretization schemes then differ in the recipe for calculating $\mathcal{E}(x)$. The first schemes for an arbitrary density of states [33, 34, 36] used a physically motivated, but otherwise ad-hoc expression

$$\mathcal{E}(x) = \frac{\int_{\epsilon(x+1)}^{\epsilon(x)} \rho(\omega) \omega d\omega}{\int_{\epsilon(x+1)}^{\epsilon(x)} \rho(\omega) d\omega}, \quad (29)$$

i.e. an average of energy weighted by $\rho(\omega)$. An improved approach was later introduced [16], where

$$\mathcal{E}(x) = \frac{\int_{\epsilon(x+1)}^{\epsilon(x)} \rho(\omega) d\omega}{\int_{\epsilon(x+1)}^{\epsilon(x)} \rho(\omega) / \omega d\omega}. \quad (30)$$

This scheme has better convergence properties as $\Lambda \rightarrow 1$ and it doesn't systematically underestimate the density of states at low energies. Neither of these two approaches, however, in general satisfies Eq. (20), which leads to artefacts which become apparent in high-resolution NRG calculations, in particular at high energies near the band edges [20]. More recently, a scheme based on solving Eq. (24) for a fixed discretization mesh was shown to be very successful in removing the most severe of these artefacts [20]. In most cases, this approach works well, it is robust and the conductance-band density of states can be reproduced accurately in numerical calculations. We find, however, that in practical NRG calculations some residual artefacts still appear, in particular in situations where the density of states has large and rapid variations. These artefacts cannot be fully removed by increasing the number of z -values used in the averaging. The artefacts appear especially near energies \mathcal{E}_j^1 , $j \in \mathbb{Z}$. Their origin can be traced back to the systematic errors in NRG calculations, which shift the spectral peaks from exact energies \mathcal{E}_j^z to $\mathcal{E}_j^z + \delta\mathcal{E}_j^z$. For given j , the error $\delta\mathcal{E}_j^z$ is a smooth function of parameter z , thus $\delta\mathcal{E}_j^{n/N_z} - \delta\mathcal{E}_j^{(n+1)/N_z}$ is a small quantity for all $n = 1, \dots, N_z - 1$. Even a narrow broadening kernel will then give a smooth final result in these energy ranges and the resolution can in principle be systematically improved by decreasing the broadening width while simultaneously increasing the total number of z values, N_z . To the contrary, the difference in the values of $\delta\mathcal{E}_j^{N_z/N_z}$ and $\delta\mathcal{E}_{j+1}^{1/N_z}$ is large, since the two calculations are based on two very different discretization meshes. This is still true even for very large N_z . Near \mathcal{E}_j^1 points, thus, there exist a minimum broadening width below which these systematic errors become unmasked and manifest themselves as sharp artefacts. This effectively limits the highest spectral resolution that one may expect to achieve in NRG calculations.

It was found that problems of this type become especially pronounced for densities of states which are very low (or zero) over considerable energy intervals. Such situation commonly occurs when NRG is used as the impurity solver in the dynamical mean-field theory [24, 25, 26]. It should be noted that a representative state will be chosen in each interval even if the interval contains very small (or even zero) spectral weight. While such states appear with little weights w_i , their presence is nevertheless found to be detrimental to the overall accuracy of the calculation. The issue is, actually, somewhat subtle: the weights w_i only affect the combination of states that forms $|f_0\rangle$. The terms $\mathcal{E}_i|i\rangle\langle i|$ in regions of small density of states still appear in H of Eq. (27) and they affect the coefficients ξ_n , t_n of the Wilson chain in a way which is detrimental for the accuracy of the calculation. This problem is especially severe for very small z , where some of the coefficients ξ_n may become very large (when expressed in units of $\Lambda^{-n/2}$).

We now study the severity of this problem on the example of a density of states with a smooth transition from lower density at high energies to higher density at lower energies. As a simple model we choose a density of states described by

$$\rho(\omega) \propto 1 + w \tanh[-a(|\omega| - \omega_0)], \quad (31)$$

where w ($0 \leq w \leq 1$) determines the height of the variation, ω_0 the energy where the change occurs and a its rapidity.

In Figs. 1 and 2 we compare $A_f(\omega)$, the spectral function on the first site of the Wilson chain (level f_0), computed using the NRG, with the model density of states $\rho(\omega)$. Calculations were performed with $N_z = 64$ z values, discretization parameter $\Lambda = 2$, truncation cutoff set at $10\omega_N$, broadening parameter $\eta = 0.01$ and patching parameter $p = 2.1$ (for details on the method see Ref. [20]). We focus now on left panels which contain results obtained using fixed grid discretization; right panels with adaptive-grid calculation results will be discussed in Sec. 4. In Fig. 1 the transition is made progressively sharper. At first only the artefacts at energies \mathcal{E}_j^1 are amplified, however for large enough a additional sharp features appear. In Fig. 2, we shift the transition point to lower energies, thereby again increasing the range of very low density of states. While for $\omega_0 = 0.9$ the artefacts are very mild, they increase significantly as soon as $\rho(\omega)$ becomes very low for large ω . It may be noted that mild artefacts may easily be removed by making the broadening kernel wider, but one then needs to renounce on obtaining high-resolution spectral functions. When artefacts are severe, they might affect even calculations with very wide broadening kernel.

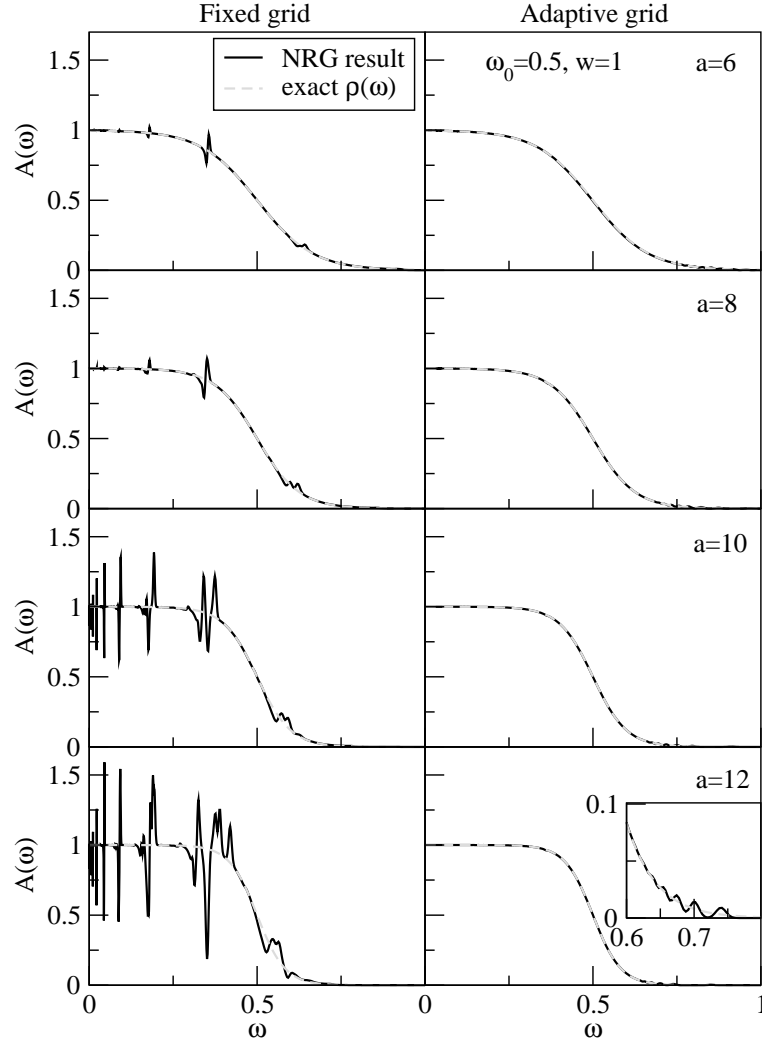


Figure 1: Spectral function of the first site on the Wilson chain for tanh density of states of the conduction band: comparison between results using fixed and adaptive discretization grids for a range of parameter a , which controls the steepness of the transition and consequently the value of $\rho(\omega)$ in the low-density range.

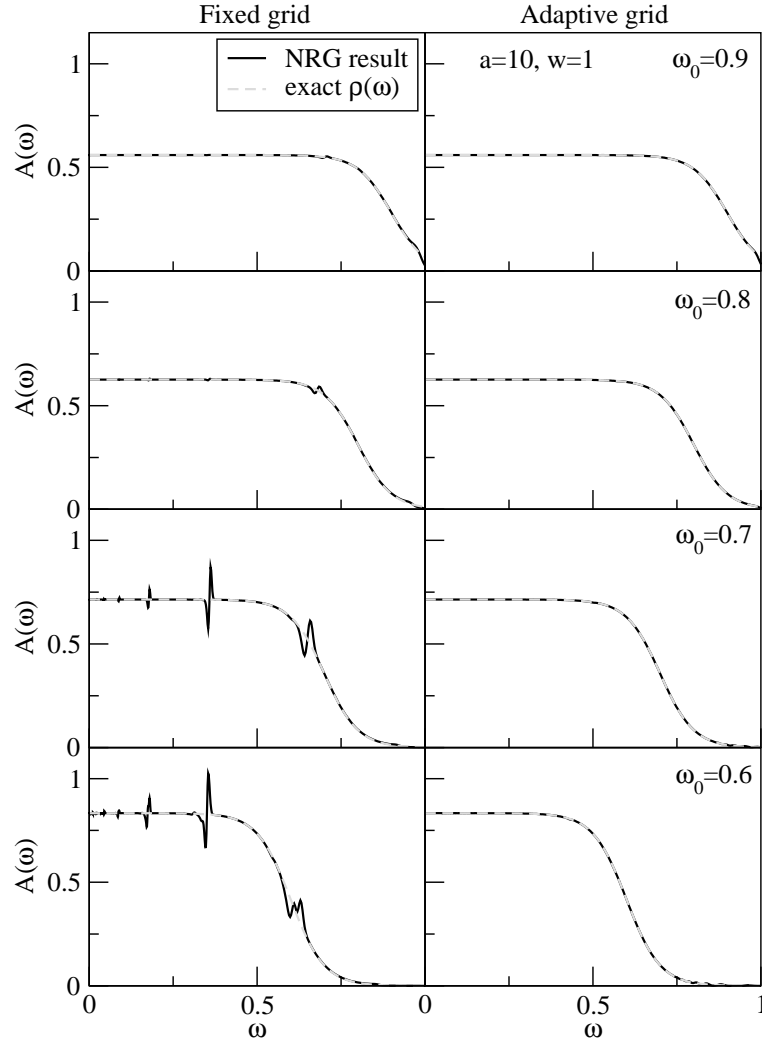


Figure 2: Spectral function of the first site on the Wilson chain for tanh density of states of the conduction band: comparison between results using fixed and adaptive discretization grids for a range of parameter ω_0 , which controls the energy of the transition from high-density to low-density range.

4. Adaptive discretization mesh

From the considerations detailed in the previous section it follows that a more appropriate choice of the discretization grid should be such that the grid were less dense in the regions of low density of states. A convenient way to implement this requirement is by demanding that the function $C(x, \epsilon)$ in Eq. (22) be of the form

$$C(x, \epsilon) = \frac{f(x)}{\rho(\epsilon)}. \quad (32)$$

It can be seen that in the limit $\rho(\epsilon) \rightarrow 0$, the corresponding energy regions will not even appear in the discretization grid, which is a very desirable property.

We consider a specialization to $f(x) \equiv A$, where A is a constant. It is easy to see that A must, in fact, be equal to the total weight $W = \int_0^1 \rho(\omega) d\omega$. We also observe that for a featureless flat band [$\rho(\omega) = 1/2$], this approach reduces to the conventional fixed discretization grid.

We furthermore note that the “characteristic energy scale at the N th NRG iteration”, ω_N , depends on the discretization grid (i.e. on function $\epsilon(x)$), thus it becomes dependent on $\rho(\omega)$. This has important consequences on the choice of parameters in NRG calculations; in particular, the truncation cutoff and the patching parameter p need to be appropriately redefined. A simple choice is to rescale ω_N by the ratio

$$R = \lim_{x \rightarrow \infty} \frac{\epsilon(x)}{\epsilon_0(x)}, \quad (33)$$

where $\epsilon_0(x)$ is the discretization grid function for fixed grid. This choice appears suitable for the tanh test functions, but it is not expected to be generally applicable. For strongly varying density of states, the patching procedure itself might become problematic and it might be better to use the complete-Fock-space approach [15, 17, 18], although that technique is not without problems either [20]. The issue of extracting spectral information from partial results at different iterations clearly merits further attention.

Comparing the right panels in Figs. 1 and 2 with the left panels, we see that the adaptive-grid approach leads to a considerable improvement; the artefacts essentially disappear. We notice that some oscillations appear in the transition region between low and high spectral density, see the inset in Fig. 1. It is important to notice that if the discretization mesh is adaptive, the width of the broadening kernel in the calculation of the continuous spectral function should ideally also take the mesh density into account; energy regions where mesh is less dense should be broadened more, since there will be less representative energy points. At the same time, one should be careful to avoid excessive broadening of spectral functions on the impurity levels, since low density in the conductance band translates into sharper features in the impurity spectral function. We note that in the extreme case of a gap in the conductance band, there might even appear delta peaks in the impurity spectral function. One should thus base the choice of the broadening width on physical considerations and on the expected spectral features.

5. Initial value problem

Both $\epsilon(x)$ and $\mathcal{E}(x)$ must have asymptotic behavior Λ^{2-x} ; this is required to obtain a logarithmic discretization around the point $x = 0$. For numerical solution of the equations, it is therefore convenient to use the following Ansatz:

$$\epsilon(x) = g(x)\Lambda^{2-x}, \quad \mathcal{E}(x) = f(x)\Lambda^{2-x}. \quad (34)$$

The unknown functions $g(x)$ and $f(x)$ are then $\mathcal{O}(1)$ for all x . The differential equations to be solved are

$$\begin{aligned} \frac{dg(x)}{dx} &= \ln \Lambda \{g(x) - C[x, g(x)\Lambda^{2-x}]\}, \\ \frac{df(x)}{dx} &= \ln \Lambda f(x) - \frac{\int_{g(x+1)\Lambda^{1-x}}^{g(x)\Lambda^{2-x}} \rho(\omega) d\omega}{\Lambda^{2-x}\rho[f(x)\Lambda^{2-x}]}, \end{aligned} \quad (35)$$

with initial conditions $g(2) = 1$ and $f(1) = 1/\Lambda$. One first solves for $g(x)$, which is then used in the equation for $f(x)$. Both equations are stiff, thus some care is needed in their numeric solution to prevent that $g(x)$ or $f(x)$ diverge.

When NRG is used as an impurity solver in the dynamical mean-field theory, the input to the calculation is the effective impurity hybridisation function which contains information on the density of states of the self-consistently defined medium. The hybridisation function usually takes the form of a tabulated function. A differential equations solver was implemented which solves for $g(x)$ and $f(x)$ on a mesh of values of x , given an arbitrary input density of states (or hybridisation function). The software package is available from the author's home page (<http://nrgljubljana.ijs.si/adapt>). For better portability the solver is written in pure ISO C++ without making use of any external libraries.

In the solver, $\rho(\omega)$ is calculated for an arbitrary point ω from the tabulated input function by linear interpolation. Integrations are performed using trapezoidal method; where the integration boundary falls inside a tabulation interval the contribution is, however, calculated by explicitly integrating the linear interpolation function. For numerical stability, it is very important that interpolation and integration be of consistent order of approximation. The differential equations are solved using fourth-order Runge-Kutta solver with adaptive reduction of the integration step size near the boundaries of the tabulation intervals. This is especially important when solving for $f(x)$ in situations where $\rho(\omega)$ has sharp features (steps, kinks, sharp peaks). In the reference implementation of the solver, we use $C(x, \epsilon) = A/\rho(\epsilon)$. Constant A is first estimated by the numerical integral $W = \int_0^1 \rho(\omega) d\omega$, but it is then refined by repeatedly solving the differential equation for $g(x)$ until $g(x)$ no longer tends to diverge; to determine a suitable value A in this shooting-method approach we use the secant method to solve the equation

$$g(x_{\max}) = \frac{A}{\rho(0)}. \quad (36)$$

When solving the differential equation for $f(x)$, it is observed that the integration steps need to be made small enough in regions of x which correspond to varying $\rho(\omega)$, otherwise $f(x)$ will diverge. For large x in the region where $\rho[f(x)\Lambda^{2-x}]$ is essentially constant, longer steps may be used.

The output from the program are tabulated functions $f(x)$ and $g(x)$ which can then be read as input to the NRG code.

6. Conclusion

A possible improvement would consist of choosing such function $C(x, \epsilon)$ to make the discretization grid denser in the regions of large variation of $\rho(\epsilon)$, in other words to make it also depend on the derivative $d\rho/d\epsilon$. Alternatively, one could systematically study the influence of various environmental modes (i.e. sets of nearby conduction-band states) on system dynamics and choose $C(x, \epsilon)$ so that sampling is denser in energy regions which contribute more [39]. Furthermore, the possibility of making the function C depend on the grid parameter x could be used to deform the mesh so that the first weight w_1^z would not be small for small z ; w_1^z tends to 0 with $z \rightarrow 0$ even if the density of states near the band edges is large, which leads to similar problems as discussed in Sec. 3, although with lesser severity.

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